Discrete Gradient θ-Methods for Port-Hamiltonian Systems

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Abstract. The paper is focused on the geometric numerical integration of port-Hamiltonian problems, via discrete gradient θ-methods. The ability of this method to retain inherent dissipativity properties of the exact dynamics is considered, as well as the stability properties of the numerical scheme with respect to a test problem based on a controlled pendulum are treated. The analysis is also equipped by selected numerical experiments.

Keywords: Port-Hamiltonian problems · Discrete gradient method · Geometric numerical integration

1 Introduction

Geometric numerical integration is nowadays a well established paradigm in Numerical Analysis, aiming to preserve qualitative and quantitative aspects of the exact dynamics along its discretization via suitable numerical schemes.

As highlighted, for instance, in [23], the denomination *geometric numerical integration* traces the vision of geometry given by Felix Klein in his outstanding Erlangen program, where he describes geometry as the study of invariants under suitable transformations. Accordingly, a numerical methods is geometric when it retains relevant properties of a dynamical system along the numerical dynamics. Building blocks of geometric numerical integration have been first placed in the scientific literature for structure-preservation in the framework of Hamiltonian problems, then conveyed to the numerical treament of evolutive problems of various kind. For a general treatment of geometric numerical methods a non-exhaustive list of relevant references is given, for instance, by [3,4,6,23,37,40,41,43,45,46,50] and references therein.

Out of Runge-Kutta methods, nearly-conserving linear multistep methods exhibiting excellent long-time behaviors have been developed [34,36,37], as well as a theory of nearly-preserving multivalue methods [9,10,29,30] and energy-preserving numerical integrators (see, for instance, [4,14] and references therein). Principles of geometric numerical integration for stochastic differential equations have also been treated in recent scientific literature, for instance in the

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conservation of invariance laws characteristic properties of stochastic oscillators [8,16,26,28,31,35,51,52,56], in nonlinear SDEs with one-sided Lipschitz drift leading to mean-square contractive dynamics [5,24,25,38], in stochastic Hamiltonian and Poisson problems [2,7,15,17,18,27,32,39,44,48,49,53] and related issues.

In this paper, we aim to focus our attention on some aspects regarding the geometric numerical integration of port-Hamiltonian problems, that are controlled systems of ODEs of fundamental importance in several fields of applications: for instance, we refer to [11,47,55,57] and references therein. As well highlighted, for instance, in [54], port-Hamiltonian dynamics is an extension of Hamiltonian canonical approach to motion, combined with the network point of view, useful in modelling and simulation of complex systems. Moreover, port-Hamiltonian systems are able to convey the interaction with their environment through specific ports, as well as to describe energy dissipation.

Under a more specific numerical point of view, it is worth preserving the peculiar dissipativity features characterizing port-Hamiltonian systems along their numerical discretization with accuracy. In particular, inspired by [13], this paper pursues the aim to study when discrete gradient θ-methods are able to retain inherent properties of the dynamics of systems with dissipation in the Hamiltonian, together with the stability properties of the numerical scheme with respect to a test problem based on a controlled pendulum. Moreover, selected numerical experiments complement the theoretical investigation.

2 Basics on Port-Hamiltonian Systems

A port-Hamiltonian problem is modelled by the following system of ODEs:

$$\begin{aligned} \dot{x} &= B(x)\nabla H(x) + G(x)u, \\ x(0) &= x_0, \\ y &= G(x)^\intercal \nabla H(x), \end{aligned} \tag{1}$$

having denoted by $x \in \mathbb{R}^n$ the state variable of the system, $u \in \mathbb{R}^m$ the input and $y \in \mathbb{R}^m$ the output. The matrix $B(x)$ is assumed to be skew-symmetric and $H(x)$ is the Hamiltonian function of the system.

Problem (1) falls in the more general framework of controlled systems of ODEs

$$\begin{aligned} \dot{x} &= f(x,u), \\ y &= h(x), \end{aligned} \tag{2}$$

whose vector field $f : \mathbb{R}^n \times \mathbb{R}^m \to \mathbb{R}^n$ is supposed to be locally Lipschitz. A relevant property for problem (2) is given by its *passivity*, occurring if there exists a continuously differentiable positive semidefinite function $V(x)$ such that

$$u^\intercal y \geq \nabla V(x)^\intercal f(x,u), \tag{3}$$

for any $(x,u) \in \mathbb{R}^n \times \mathbb{R}^m$. The function $V(x)$ is denoted as *storage function*. If (3) is satisfied as an equality, the system is said to be *lossless*, i.e., $u^\intercal y = \dot{V}$.

We observe that the condition of passivity can be recast in integral form. Indeed, side-by-side integrating Equation (3) yields

$$\langle y, u\rangle_{L^2} \geq V(t) - V(0),$$

for any $t \geq 0$, with

$$\langle y, u\rangle_{L^2} = \int_0^t y^\intercal u ds.$$

One can easily check that system (1) is lossless with respect to the Hamiltonian function as storage function. Indeed,

$$\begin{aligned}\dot{H} &= \nabla H(x)^\intercal \dot{x} \\ &= \nabla H(x)^\intercal B(x)\nabla H(x) + \nabla H(x)^\intercal G(x)u.\end{aligned}$$

Since $\nabla H(x)^\intercal B(x)\nabla H(x) = 0$, due to the skew-symmetry of $B(x)$, we have

$$\dot{H} = \nabla H(x)^\intercal G(x)u = y^\intercal u.$$

Then, in terms of L^2 product, the property of lossless with respect to the Hamiltonian function reads as

$$\langle y, u\rangle_{L^2} = H(t) - H(0).$$

3 Discrete Gradient θ-Methods

Following [13], we use a first order discretization of the gradient, defined as

$$\overline{\nabla} H(x_n, x_{n+1})^\intercal (x_{n+1} - x_n) = H(x_{n+1}) - H(x_n).$$

Correspondingly, we introduce the following discrete gradient θ-method of problem (1)

$$\begin{aligned} x_{n+1} &= x_n + h(1-\theta)\Big(B(x_n)\overline{\nabla} H(x_{n-1}, x_n) + G(x_n)u_n\Big) \\ &\quad + h\theta\Big(B(x_{n+1})\overline{\nabla} H(x_n, x_{n+1}) + G(x_{n+1})u_{n+1}\Big), \\ y_{n+1} &= G(x_{n+1})^\intercal \overline{\nabla} H(x_n, x_{n+1}), \end{aligned} \tag{4}$$

over the grid of equispaced points

$$\mathcal{I}_h = \left\{ t_n = nh, \quad n = 0, 1, \ldots, N, \quad h = \frac{T}{N} \right\},$$

supposing that $[0, T]$ is the selected time window.

Let us compute $\overline{\nabla} H(x_n, x_{n+1})^\intercal (x_{n+1} - x_n)$, using the hyphotesis of skew-simmetry for the matrix $B(x)$:

$$\overline{\nabla} H(x_n, x_{n+1})^\intercal (x_{n+1} - x_n) = h(1-\theta)\Big(\overline{\nabla} H(x_n, x_{n+1})^\intercal B(x_n) \overline{\nabla} H(x_{n-1}, x_n) + \overline{\nabla} H(x_n, x_{n+1})^\intercal G(x_n) u_n\Big) + h\theta y_{n+1}^\intercal u_{n+1}.$$

We aim to satisfy, along the numerical dynamics, a discrete balance law, i.e., we aim to express the Hamiltonian deviation $\Delta H(x_{n+1}) = H(x_{n+1}) - H(x_n)$ as a quantity proportional to $y_{n+1}^\intercal u_{n+1}$.

For $\theta = 1$, we have

$$\overline{\nabla} H(x_n, x_{n+1})^\intercal (x_{n+1} - x_n) = h y_{n+1}^\intercal u_{n+1},$$

i.e., the only θ-method satisfying a discrete balance law is the implicit Euler method. For all other θ-methods with $\theta \neq 1$, the defect is equal to

$$h(1-\theta)\Big(\overline{\nabla} H(x_n, x_{n+1})^\intercal B(x_n) \overline{\nabla} H(x_{n-1}, x_n) + y_n^\intercal u_n\Big)$$

and, under suitable regularity, it can be negligible in a left neighborhood of $\theta = 1$, where unconditionally stability is also acknowledgeable.

Let us consider as test problem the port-Hamiltonian controlled pendulum [13], i.e., problem (1) with

$$B = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}, \quad G = \begin{bmatrix} 0 \\ 1 \end{bmatrix}, \quad H(q,p) = \frac{p^2}{2} + 1 - \cos(q),$$

and input $u(y) = -\alpha \arctan(y)$, with $\alpha > 0$, leading to

$$\begin{bmatrix} \dot{q} \\ \dot{p} \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \begin{bmatrix} -\sin(q) \\ p \end{bmatrix} - \begin{bmatrix} 0 \\ \alpha \arctan(p) \end{bmatrix}. \tag{5}$$

Figs. 1 and 2 show the corresponding solution orbits, arising from the numerical dynamics of (4) for selected values of θ and α. One can appreciate that the choices of the parameters θ and α have a direct influence on the stability of the numerical dynamics, that deserves being properly analyzed.

4 Stability Issues

Let us perform the analysis of stability of the numerical scheme (4), assuming as discrete gradient operator the averaged vector field discrete gradient, i.e.,

$$\overline{\nabla} H(x_n, x_{n+1}) = \int_0^1 \nabla H(\rho(\alpha)) \mathrm{d}\alpha,$$

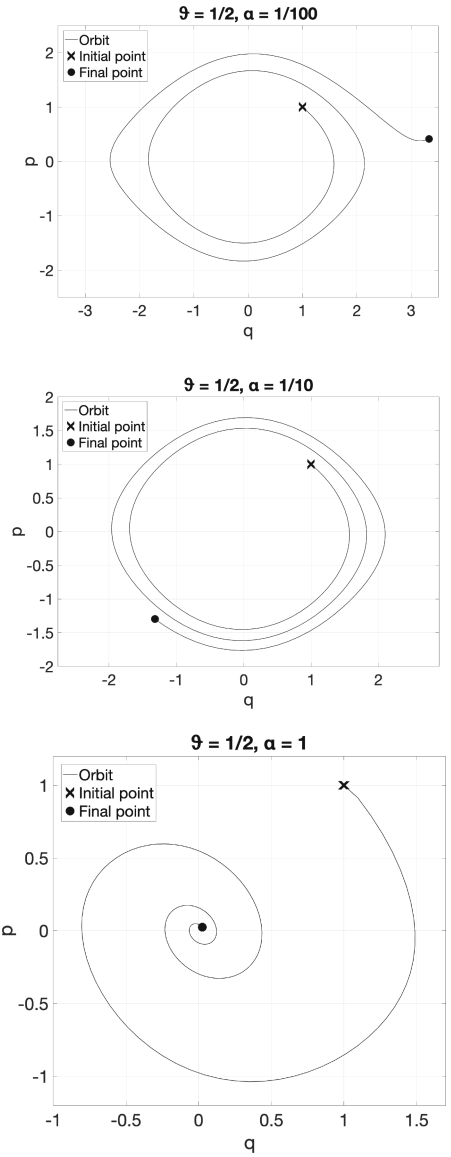

Fig. 1. Solution orbits related to the controlled pendulum (5) with the discrete gradient θ-method (4), for the highlighted values of θ and α.

with $\rho(\tau) = x_n(1-\tau) + x_{n+1}\tau$. For the approximation of the integral, we use the trapezoidal rule, i.e.,

$$\overline{\nabla} H(x_n, x_{n+1}) \approx \frac{1}{2} \left(\nabla H(x_{n+1}) + \nabla H(x_n) \right).$$

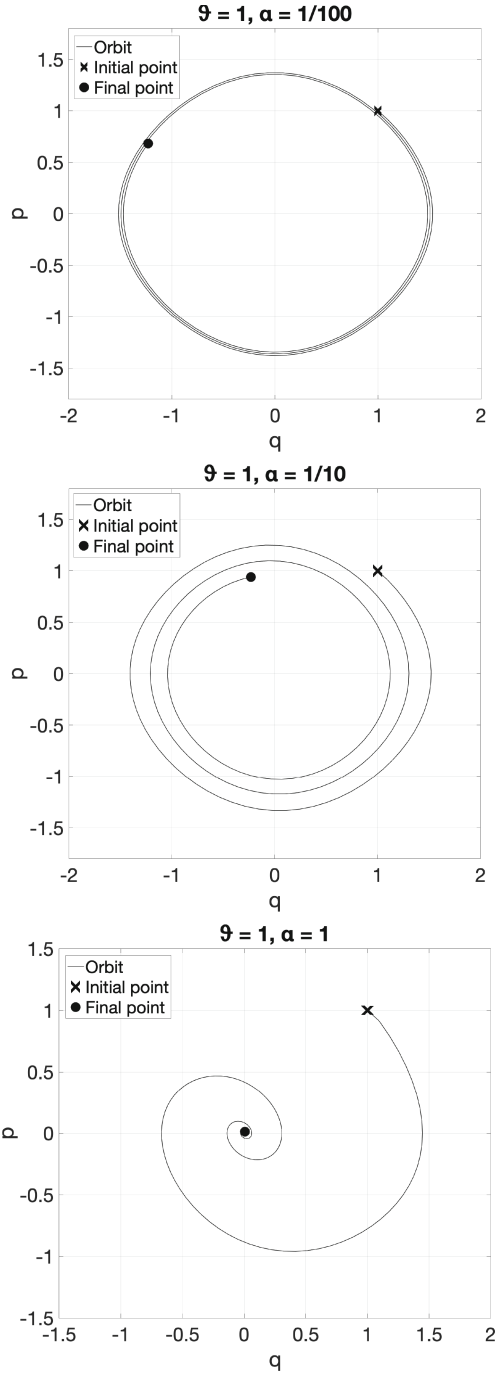

Fig. 2. Solution orbits related to the controlled pendulum (5) with the discrete gradient θ-method (4), for the highlighted values of θ and α.

We consider as test problem the port-Hamiltonian controlled pendulum (5). Considering that, in this case,

$$\overline{\nabla} H(x_n, x_{n+1}) \approx \frac{1}{2} \begin{bmatrix} \sin(q_{n+1}) + \sin(q_n) \\ p_{n+1} + p_n \end{bmatrix},$$

applying the discrete gradient θ-method (4) to the controlled pendulum (5) leads to

$$\begin{bmatrix} q_{n+1} \\ p_{n+1} \end{bmatrix} = \begin{bmatrix} q_n \\ p_n \end{bmatrix} + \frac{h}{2}(1-\theta) \begin{bmatrix} p_n + p_{n-1} \\ -\sin(q_{n-1}) - \sin(q_n) - \alpha \arctan(p_n) \end{bmatrix} + \frac{h}{2}\theta \begin{bmatrix} p_{n+1} + p_n \\ -\sin(q_n) - \sin(q_{n+1}) - \alpha \arctan(p_{n+1}) \end{bmatrix}.$$

Since $p_{n+1} = p_n + \mathcal{O}(h)$ and $q_{n+1} = q_n + \mathcal{O}(h)$ and via local linearization of the circular functions in last equation, we obtain

$$\begin{bmatrix} q_{n+1} \\ p_{n+1} \end{bmatrix} = \begin{bmatrix} q_n \\ p_n \end{bmatrix} + \frac{h}{2}(1-\theta) \begin{bmatrix} p_n + p_{n-1} \\ -q_{n-1} - q_n - \alpha p_n \end{bmatrix} + \frac{h}{2}\theta \begin{bmatrix} p_{n+1} + p_n \\ -q_n - q_{n+1} - \alpha p_{n+1} \end{bmatrix} + \mathcal{O}(h^2).$$

Neglecting the remainder term $\mathcal{O}(h^2)$, the aforestated equation is a system of second order difference equations, that we can write in compact form as

$$x_{n+1} = Ax_n + Bx_{n-1}, \tag{6}$$

with

$$A = \frac{1}{h^2\theta^2 + 2\alpha h\theta + 4} \begin{bmatrix} h^2\theta(\theta-1) + 4h\theta\alpha + 4 & h\left(\alpha h\theta^2 + 2\theta + 2\right) \\ -4h(\theta+1) & -h^2\theta + 2\alpha h(\theta-1) + 4 \end{bmatrix},$$

$$B = \frac{h(\theta-1)}{h\theta\left(2\alpha + h\theta\right) + 4} \begin{bmatrix} h\theta & -h\theta\alpha - 2 \\ 2 & h\theta \end{bmatrix}, \qquad x_n = \begin{bmatrix} q_n \\ p_n \end{bmatrix}.$$

Let us recast Eq. (6) as a system of first order difference equations, by employing the auxiliary discrete state variable $z_n = x_{n-1}$, leading to

$$\begin{bmatrix} x_{n+1} \\ z_{n+1} \end{bmatrix} = C \begin{bmatrix} x_n \\ z_n \end{bmatrix}, \qquad C = \begin{bmatrix} A & B \\ I & \mathbf{0} \end{bmatrix}, \tag{7}$$

being I the 2×2 identity matrix and $\mathbf{0}$ the zero matrix of the same dimension.

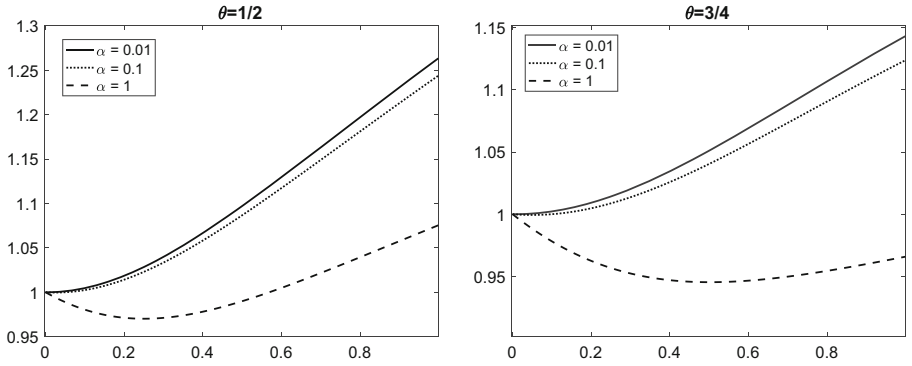

Fig. 3. Stability radii of the matrix C in (7) with respect to the stepsize, for the highlighted values of θ and α.

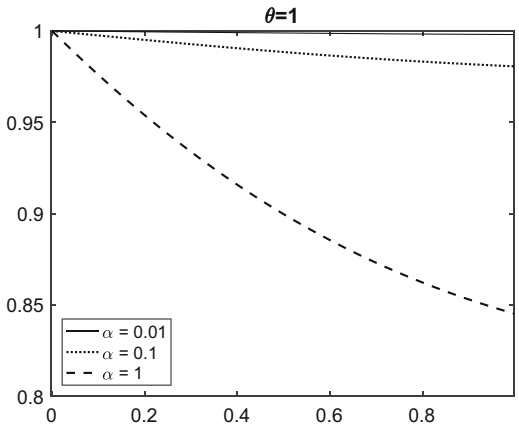

Fig. 4. Stability radii of the matrix D in (8) with respect to the stepsize, for $\theta = 1$ and selected values of α.

A degenerate case occurs for $\theta = 1$ since, in correspondence of this value, the matrix B is the zero matrix and, as a consequence, the second order system (6) reduces to the first order system of difference equations $x_{n+1} = Dx_n$, with

$$D = \frac{1}{h(2\alpha + h) + 4} \begin{bmatrix} 4(\alpha h + 1) & h\,(\alpha h + 4) \\ -8h & 4 - h^2 \end{bmatrix}. \tag{8}$$

Stability radii of the matrices C and D are depicted in Figs. 3 and 4, for selected values of θ and α and depicted as functions of h. As visible, for $\theta = \frac{1}{2}$, the stability radius is smaller than 1 only for selected values of α and for h satisfying a restriction. For $\theta = \frac{3}{4}$, larger values of α lead to a stable pattern, considering the stability radius behaviour displayed in Fig. 3, without stepsize restrictions. For $\theta = 1$, the behaviour displayed in Fig. 4 shows unconditional

stability, since the spectral radius is always smaller than 1, even if it goes closer and closer to 1 for smaller values of α. Indeed, for α tending to 0, both matrices C and D in (7) and (8) tends to the identity matrix.

It is also worth observing that the unstable behaviour of the matrix C for small values of α is also coherent with the corresponding phase portraits shown in Figs. 3 and 4.

5 Concluding Remarks

We have focused our attention on the geometric numerical integration of port-Hamiltonian problems, assuming that the exact dynamics is approximated by means of the discrete gradient θ-method. In particular, the analysis has revealed the ability of this method in numerically retaining peculiar dissipativity features of the problem, such as a discrete balance law. In other terms, the discrete gradient θ-method provides Hamiltonian deviations $\Delta H(x_{n+1})$ proportional to $y_{n+1}^{\intercal} u_{n+1}$.

The analysis has also included the investigation of some stability issues for the discrete gradient θ-method, given with respect to the controlled pendulum. Stability properties have then been given in terms of spectral properties of the involved stability matrices, highlighting their connection with the value of the parameter θ characterizing the method and additional parameters visible in the problem.

This research may be extended to the geometric numerical integration of many significant evolution problems exhibiting peculiar dissipative dynamics, such as deterministic and stochastic reaction-diffusion problems or non-local problems described by integral and fractional differential equations. [1,12,19–22,33,42].

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